

Methyl hexanedioate
627-91-8 | DTXSID9044451

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 12.3 °C

Global applicability domain: Inside

Local applicability domain index: 8.69e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

Image not found

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Measured: 9.00

Predicted: 12.3